**IMPACT: Journal of Computational Sciences and Information Technology (IMPACT: JCSIT)**
**ISSN(P): Applied; ISSN(E): Applied**
**Vol. 1, Issue 1, Dec 2016, 19-28**


# A SEARCH FOR NATURAL ANALOGS OF PSORALEN INVOLVED IN THE TREATMENT OF VITILIGO: A COMPUTATIONAL APPROACH

**SUJATHA, P L[1], KUMARASAMY, P[2], PREETHA S P[3] & BALACHANDRAN C[4]**

[1]College of Food and Dairy Technology, Koduvalli, Chennai, Tamil Nadu, India

[2]Department of Bioinformatics, Madras Veterinary College, Chennai, Tamil Nadu, India

[3]Department of Veterinary Pharmacology, Madras Veterinary College, Chennai, Tamil Nadu, India

[4]The Dean, Madras Veterinary College, Chennai, Tamil Nadu, India

## ABSTRACT

Vitiligo is an acquired skin disease which includes patterned loss of melanin pigment due to destruction of melanocytes. Vitiligo associated protein-1, also called as F-box only protein 11 is responsible for this disease which is encoded by a gene VIT-1 located at the chromosome 2p16 position. The so far known drug compound to inhibit this protein is psoralen. Similar structural natural compounds were selected to study the inhibition of the protein like Ginko-Biloba (maidenhair tree leaves), Turmeric (Curcumin), khella (Ammivisnaga). Analogue search is done for each natural compound and virtual screening was performed for all analogs (300) from which best 5 lead compounds were selected using Argus Lab. Further with resultant lead compounds docking is performed with the target protein using Discovery Studio 4.0. Best analogue from each natural compound was selected by their binding energy values. Since the compounds are only modified variants of natural template molecules, they may be presumed to have more activity but less toxicity compared to their counterparts in modern medicine. The product(s) is thus envisaged to be better variant(s) of existing natural molecule(s) designed using bioinformatics tools and semi-synthetically prepared under laboratory conditions for further testing and validation as potential drug candidates.

**KEYWORDS:** Vitiligo, Psoralen, Virtual Screening, Analogs, Interaction Studies